

Tuning phase transition between quantum spin Hall and ordinary insulating phases

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An effective theory is constructed for analyzing a generic phase transition between the quantum spin Hall and the insulator phases. Occurrence of degeneracies due to closing of the gap at the transition are carefully elucidated. For systems without inversion symmetry the gap-closing occurs at $\pm \vec{k}_0 (\neq \vec{G}/2)$ while for systems with inversion symmetry, the gap can close only at wave-numbers $\vec{k} = \vec{G}/2$, where \vec{G} is a reciprocal lattice vector. In both cases, following a unitary transformation which mixes spins, the system is represented by two decoupled effective theories of massive two-component fermions having masses of opposite signs. Existence of gapless helical modes at a domain wall between the two phases directly follows from this formalism. This theory provides an elementary and comprehensive phenomenology of the quantum spin Hall system.

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I. INTRODUCTION

The intrinsic spin Hall effect (SHE)^{1,2} driven by the relativistic spin-orbit interaction and the associated Berry curvature of the Bloch wavefunctions attracts considerable attention both theoretically and experimentally. In conducting materials such as doped GaAs, the external electric field produces transport current and dissipation, even though the spin current transverse to it is dissipationless. Therefore it is highly desirable to design systems showing the SHE without dissipation. Spin Hall insulator (SHI) has been proposed for this purpose by some of the present authors, and its candidate materials are HgTe, PbTe, α -Sn and so forth³. These band insulators are predicted to show finite spin Hall conductivity σ_H^s , which is not quantized and depends on parameters in the model Hamiltonian. Later it has been realized that gapless edge modes in semi-infinite systems do not exist in generic cases. These two features, i.e., the non-quantized σ_H^s and the absence of gapless edge modes, are closely related to the absence of conserved spin current in the presence of spin-orbit interaction, i.e., there is no U(1) gauge symmetry for spin current. Therefore it was difficult to distinguish between the SHI and usual insulators.

Recently, Kane and Mele proposed a model for time-reversal (T-) invariant systems^{4,5}, which manifests a finite SHE and demonstrated its distinction from an ordinary insulator due to the topological nature of its ground state. The pertinent Z_2 topology is represented by an integer Δ defined for Bloch wavefunctions in the bulk, whose parity distinguishes the relevant phases. Physically, Δ is identical with the number of pairs of helical edge modes. In a system with $\Delta = \text{odd}$, referred to

as quantum spin Hall (QSH) system^{4,5,6,7,8,9,11,12,13,14,15}, the odd number of pairs of helical edge modes is robust against weak nonmagnetic disorder and interactions^{16,17}. When $\Delta = \text{even}$, gapless edge modes can hybridize each other and a gap will open even at the edge. The system is then referred to as spin Hall insulator (SHI). Transitions between phases with $\Delta = \text{even}$ (SHI) and $\Delta = \text{odd}$ (QSH) occur only when the gap is closed by tuning parameters of the model. Constructing a theory for analyzing these transitions is a challenge of paramount interest.

In this paper, we develop an effective continuum theory for phase transitions between QSH and SHI systems in 2D and discuss (i) classification of the possible types of transition, (ii) existence of gapless helical edge modes, and (iii) the change of the Z_2 topological number at the transition. The basic idea is that effective continuum theory focusing on the vicinity of the gap-closing points at the transition can be constructed even though characterization of each phase requires information over the whole first Brillouin zone. Namely, the *change* across the phase boundary is much easier to elucidate, and the relation between the topological number and the helical edge modes is rather transparent. This work concerns local features in \vec{k} space, and is complementary to Refs. 5,26, which treats global topological structure in \vec{k} space. We ignore interaction and disorder effect in this paper, since the robustness of the system is inferred from the topological stability.

II. GAP CLOSING AT THE PHASE TRANSITION

Since the phase transition necessarily accompanies closing of the gap^{5,9,10}, we commence with an analysis of generic gap-closing in a two-dimensional (2D) gapped spin-1/2 T-symmetric system with spin-orbit interaction. A Hamiltonian matrix for Bloch wavefunctions can be written in a block form,

$$H(\vec{k}) = \begin{pmatrix} h_{\uparrow\uparrow}(\vec{k}) & h_{\uparrow\downarrow}(\vec{k}) \\ h_{\downarrow\uparrow}(\vec{k}) & h_{\downarrow\downarrow}(\vec{k}) \end{pmatrix}. \quad (1)$$

The dimension of the matrix $h_{\sigma\sigma'}(\vec{k})$ depends on systems considered; nevertheless, in order to describe the phase transition, it is sufficient to restrict the dimension of the matrices $h_{\sigma\sigma'}(\vec{k})$ to be one or two, as we will see later. To investigate the topological order of the Hamiltonian, its spectrum is assumed to have a gap, within which the Fermi energy lies. The T-symmetry is represented by the operator, $\Theta = i\sigma_y K$ ($\sigma_{x,y,z}$ are Pauli matrices and K stands for complex conjugation). For $H(\vec{k})$ it implies,

$$H(\vec{k}) = \sigma_y H^T(-\vec{k}) \sigma_y, \quad (2)$$

or, equivalently, $h_{\uparrow\uparrow}(\vec{k}) = h_{\uparrow\downarrow}^T(-\vec{k})$ and $h_{\uparrow\downarrow}(\vec{k}) = -h_{\downarrow\uparrow}^T(-\vec{k})$. This, in turn, results in a degeneracy between states at \vec{k} and $-\vec{k}$, forming Kramers pairs.

Tuning some parameters in the Hamiltonian may drive a transition, where the gap closes and degeneracies between the valence and the conduction bands occur at certain wavevectors $\vec{k} = (k_x, k_y)$. To pursue the phase transition, we will focus on “generic” gap-closing achieved by tuning a *single* parameter m . (For mere convenience, the critical value of m for which a generic gap-closing occurs is chosen as $m = 0$.) Non-generic gap-closing achieved by tuning *several* parameters are excluded in our analysis. This is because such kind of gap-closing can be circumvented by small perturbation, meaning that it cannot be associated with a phase transition. As we show below, generic gap-closing are classified into two cases shown schematically in Fig. 1 (a)(b) (depending on symmetry under parity). We note that while we have not made any assumption on the Z_2 topological number, both cases (a) and (b) turn out to encode quantum phase transitions between the QSH and the SHI phases. Among the known models describing this kind of phase transition, the Kane-Mele model on the honeycomb lattice⁵ falls within class (a) while the HgTe quantum well model¹⁸ belongs to class (b).

The QSH-SHI phase transitions pertaining to Fig. 1 (a)(b) are not so trivial as it might look. In general, energy levels repel each other, thereby the valence and the conduction bands do not touch when the number of tuned parameters is not large enough. The number of tuned parameters to achieve degeneracy, called the codimension, is sensitive to the symmetry and the dimension

of the system considered. For example, in three dimensions the gap-closing of the type (a) in Fig. 1 does not occur¹⁹.

Consider now a spatial inversion (I)-symmetry which plays an important role beside T-symmetry. The former requires the relation $\varepsilon_{n\alpha}(\vec{k}) = \varepsilon_{n\alpha}(-\vec{k})$, while the latter implies $\varepsilon_{n\alpha}(\vec{k}) = \varepsilon_{n\bar{\alpha}}(-\vec{k})$, where $\varepsilon_{n\alpha}(\vec{k})$ is the energy of band n with pseudospin α , and $\bar{\alpha}$ is the pseudospin opposite to α ²⁰. If both symmetries are respected, $\varepsilon_{n\alpha}(\vec{k}) = \varepsilon_{n\bar{\alpha}}(\vec{k})$ and there is a Kramers double degeneracy at each \vec{k} . If I-symmetry is broken, double degeneracy occurs at points $\vec{k} = -\vec{k} + \vec{G}$, i.e. $\vec{k} = \vec{k}_i \equiv \vec{G}/2$, where \vec{G} is a reciprocal lattice vector; no double degeneracy occurs at other points (unless an additional symmetry is present). The I-asymmetric and I-symmetric cases are therefore considered separately below.

A. Inversion asymmetric systems

In this case, when $\vec{k} \neq -\vec{k} + \vec{G}$, each band is *non-degenerate*, and the gap between two bands can close at some points \vec{k} . At the gap-closing point, one valence band and one conduction band become degenerate. The codimension is three²¹. This codimension three is equal to the number of parameters involved, that is, k_x , k_y and m . Thus the gap can close at some \vec{k} when the parameter m is tuned to a critical value.

On the other hand, when $\vec{k} = -\vec{k} + \vec{G}$, the band is doubly degenerate, and the codimension is five^{22,23}, exceeding the number of tunable parameters which is one (that is, m). Thus, generic gap-closing cannot occur at $\vec{k} = \vec{G}/2$ ²⁴.

We thus focus on the case $\vec{k} \neq \vec{G}/2$. Near the gap-closing point $\vec{k} = \vec{k}_0 (\neq \vec{G}/2)$, the system’s Hamiltonian corresponds to massive two-component fermion, and can be expressed as $\mathcal{H} = m\sigma_z + (k_x - k_{0x})\sigma_x + (k_y - k_{0y})\sigma_y$ (after unitary and scale transformations). T-symmetry requires that the gap closes simultaneously at \vec{k}_0 and $-\vec{k}_0$ as depicted in Fig. 1 (a), and that the masses at $\vec{k} = \pm\vec{k}_0$ have opposite signs. In the honeycomb-lattice model for QSH^{4,5} the gap closes at the K, K' points; Hence it reduces to the present scheme without I-symmetry.

B. Inversion symmetric systems

In this case, the energies are doubly degenerate at each \vec{k} . At the phase transition, the gap between the two doubly-degenerate bands closes. Hence, we consider 4×4 Hamiltonian matrix $H(\vec{k})$ ($h_{\alpha\beta}(\vec{k})$ in Eq. (1) are 2×2). The I-symmetry is imposed as

$$H(-\vec{k}) = PH(\vec{k})P^{-1}, \quad u(-\vec{k}) = Pu(\vec{k}), \quad (3)$$

where P is a unitary matrix independent of \vec{k} , and $u(\vec{k})$ is the periodic part of the Bloch wavefunction: $\varphi_{\vec{k}}(\vec{r}) =$

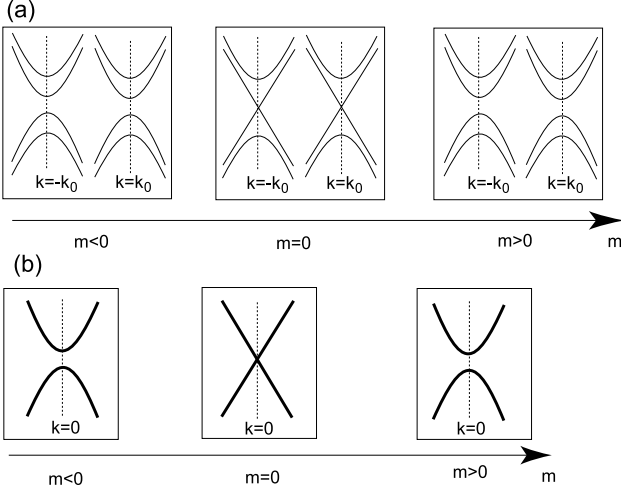


FIG. 1: Generic gap-closing for (a) inversion-asymmetric and (b) inversion-symmetric cases. In case (b) all the states are doubly degenerate by Kramers theorem.

$u(\vec{k})e^{i\vec{k}\cdot\vec{r}}$. As the inversion does not flip spin, this unitary matrix P should be block-diagonal in spin space:

$$P = \begin{pmatrix} P_{\uparrow} & \\ & P_{\downarrow} \end{pmatrix}. \quad (4)$$

In fact, all cases reduce to a case $P_{\uparrow} = P_{\downarrow} = \text{diag}(\eta_a, \eta_b)$ with $\eta_a = \pm 1$, $\eta_b = \pm 1$, as can be shown directly by applying a unitary transformation. η_a and η_b represent the parity eigenvalues of the atomic orbitals.

Occurrence of gap closing turns out to be different for the cases (i) $\eta_a = \eta_b$ and (ii) $\eta_a = -\eta_b$. The case (i) $\eta_a = \eta_b = \pm 1$ is realized when the atomic orbitals a , b have the same parity, such as two s -like orbitals or two p -like orbitals. The ensuing constraints on the Hamiltonian are: $h_{\uparrow\uparrow} = h_{\downarrow\downarrow}^T$ is an even function of \vec{k} , and $h_{\uparrow\downarrow} = h_{\downarrow\uparrow}^{\dagger}$ is an antisymmetric matrix, even function in \vec{k} . In an explicit form, the generic Hamiltonian becomes

$$H(\vec{k}) = E_0(\vec{k}) + \sum_{i=1}^5 a_i(\vec{k})\Gamma_i \quad (5)$$

where a_i 's and E_0 are real even functions of \vec{k} . Γ_i are 4×4 matrices given by $\Gamma_1 = 1 \otimes \tau_x$, $\Gamma_2 = \sigma_z \otimes \tau_y$, $\Gamma_3 = 1 \otimes \tau_z$, $\Gamma_4 = \sigma_y \otimes \tau_y$, and $\Gamma_5 = \sigma_x \otimes \tau_y$, where σ_i and τ_i are Pauli matrices acting on spin and orbital spaces, respectively. The Eigenenergies are given by $E_0 \pm \sqrt{\sum_{i=1}^5 a_i^2}$. The gap closes when $a_i(\vec{k}) = 0$ for $i = 1, \dots, 5$. It means that the codimension is five, the same as in the case at $\vec{k} = \vec{G}/2$ without I-symmetry. Thus there are no solutions of k_x , k_y and m which satisfy these five relations. The gap never closes in this case.

Next we consider the case $\eta_a = -\eta_b = \pm 1$, i.e. $P = \eta_a \tau_z = \pm \tau_z$, where the two constituent atomic orbitals

have different parity. The Hamiltonian reads,

$$H(\vec{k}) = a_0(\vec{k}) + a_5(\vec{k})\Gamma'_5 + \sum_{i=1}^4 b^{(i)}(\vec{k})\Gamma'_i \quad (6)$$

where $a_0(\vec{k})$ and $a_5(\vec{k})$ are even functions of \vec{k} , and $b^{(i)}(\vec{k})$ are odd functions of \vec{k} . Here Γ'_i are 4×4 matrices given by $\Gamma'_1 = \sigma_z \otimes \tau_x$, $\Gamma'_2 = 1 \otimes \tau_y$, $\Gamma'_3 = \sigma_x \otimes \tau_x$, $\Gamma'_4 = \sigma_y \otimes \tau_x$, and $\Gamma'_5 = 1 \otimes \tau_z$. In this case the gap closes only when five equations $a_5(\vec{k}) = 0$, $b^{(i)}(\vec{k}) = 0$ are satisfied. For a generic point \vec{k} with $\vec{k} \neq \vec{G}/2$, these five equations cannot be satisfied simultaneously, through a change of a single parameter²⁵. On the other hand, at the high-symmetry points $\vec{k} = \vec{k}_i = \vec{G}/2$, the situation is different. At these points the odd functions $b^{(i)}(\vec{k})$ vanish identically, and one has only to tune $a_5(\vec{k})$ to be zero. Thus, the gap closes by fine-tuning a single parameter. To be more specific, we take $\vec{k} = 0$ as an example, and write down the Hamiltonian explicitly. Extension to other $\vec{k} = \vec{G}/2$ points is straightforward. The Hamiltonian is expanded to linear order in \vec{k} as

$$H(\vec{k}) \sim E_0 + m\Gamma'_5 + \sum_{i=1}^4 \left(\vec{\beta}^{(i)} \cdot \vec{k} \right) \Gamma'_i, \quad (7)$$

where E_0 and m are constants, and $\vec{\beta}^{(i)}$ ($i = 1, \dots, 4$) are two-dimensional real constant vectors. Further simplification is obtained after judicious unitary transformations. The Hamiltonian finally acquires the block-diagonal form,

$$H(\vec{k}) = E_0 + \begin{pmatrix} m & z_- & & \\ z_+ & -m & & \\ & & m & -z_+ \\ & & -z_- & -m \end{pmatrix}. \quad (8)$$

where $z_{\pm} = b_1 k_x + b_3 k_y \pm i b_2 k_y$ with real constants b_1 , b_2 and b_3 . Note that in materials with high crystallographic symmetry (e.g tetragonal), one has $b_1 = b_2$ and $b_3 = 0$, leading to $z_{\pm} \propto k_x \pm i k_y$. We have thus demonstrated a feature: *The Hamiltonian of a generic system with spin-orbit coupling obeying T- and I- symmetries decouples, after an appropriate choice of basis, into a pair of Hamiltonians describing two-component fermions with opposite sign of the corresponding mass terms.* (Such decoupling is expected in the special case where s_z is a good quantum number, since the system describes two copies of a quantum Hall system). Experimental consequences are immediate as the Hamiltonian (8) is equivalent to the one suggested for the HgTe quantum well in Ref. 18 (based on phenomenological arguments). Gap closing at $\vec{k} = 0$ when the parameter m is tuned to zero is now obvious, since the eigenenergies are $E = E_0 \pm \sqrt{m^2 + z_+ z_-}$. The inversion matrix in this basis is written as $\eta_a \otimes \tau_z = \eta_a \text{diag}(1, -1, 1, -1)$.

Summing up to this point, we discussed generic types of gap closing in time-reversal invariant systems, achieved

by tuning a single parameter. Taking I-symmetry into consideration, two types of gap-closing scenarios have been found: (a) simultaneous gap closing at $\vec{k} = \pm\vec{k}_0 \neq \vec{G}/2$ occur in systems without I-symmetry, and (b) gap closing between two Kramers-degenerate bands (i.e. four bands) at $\vec{k} = \vec{G}/2$ occur in systems with I-symmetry (see Fig. 1). Due to the level repulsion, the gap-closing by tuning a single parameter occurs only in limited cases. We will see in the subsequent discussion that these cases of gap-closing exactly coincides with the phase transition between the QSH and the insulating phases. In this sense our theory characterizes the QSH phase from the local features in \vec{k} space.

C. Change of the Z_2 topological number at the gap-closing point

Now we focus on the change of Z_2 topological number at the gap closing, assuming that except for the gap closing ($m = 0$) the bands are fully gapped. Hence, both phases at $m > 0$ and $m < 0$ are band insulators, and have well-defined Z_2 topological numbers. For the I-symmetric case (a), the homotopy characterization in Ref. 26 is applicable; for the lower band at the critical value $m = 0$, there is one vortex at \vec{k}_0 and one antivortex at $-\vec{k}_0$. Thus, when the parameter m is tuned across $m = 0$, the Chern number for the whole contracted surface²⁶ changes by one. Thus, the Z_2 topological numbers are different by one for the $m > 0$ and the $m < 0$ sides. One of the phases is the QSH phase, while the other is the SHI. For the I-symmetric case (b), Fu and Kane¹³ developed a simple method to calculate the Z_2 topological number Δ as

$$(-1)^\Delta = \prod_{i=1}^4 \prod_{m=1}^N \xi_{2m}(\vec{k}_i), \quad (9)$$

where \vec{k}_i are the four high-symmetry points satisfying $\vec{k} = \vec{G}/2$, $\xi_{2m}(k_i)$ is the parity eigenvalue at each of these

points, and N is the number of Kramers pairs below E_F . In the present case the gap at $\vec{k} = 0$ collapses when $m = 0$. Hence only the parity eigenvalue at $\vec{k} = 0$ can change at the phase transition. Since the inversion matrix is given by $P = \eta_a \otimes \tau_z = \eta_a \sigma_0 \otimes \tau_z$, the parity eigenvalues are $-\eta_a (= \eta_b)$ and $+\eta_a$ for the lower-band states at $m > 0$ and $m < 0$, respectively. Hence, the parity eigenvalue changes sign, and the Z_2 topological number Δ changes by one. Thus, on the two sides of the band touching, $m > 0$ and $m < 0$, one of the phases is the QSH phase, while the other one is the simple insulator (SHI) phase.

III. HELICAL EDGE STATES

Let us regard the usual insulating phase as our vacuum, so that the domain wall between the QSH phase and the insulating phase is the edge of the sample. Such a domain wall is described by a spatially dependent mass parameter $m(x)$ satisfying $m(\pm\infty) = \pm m_0$, i.e.,

$$m = \begin{cases} m_0 & : x \gg 0 \\ -m_0 & : x \ll 0. \end{cases} \quad (10)$$

We do not specify the detail of the crossover between m_0 and $-m_0$, because it is not important for the subsequent discussions. For Fig. 1(a), one can consider the Weyl fermions at $\vec{k} = \pm\vec{k}_0$ separately. Masses of these Weyl fermions change sign at $m = 0$; hence they yield the edge states localized at the domain wall, as explained in Ref. 27. Because the Weyl fermions at $\vec{k} = \pm\vec{k}_0$ are related to each other by time-reversal symmetry, the two edge states form a Kramers pair.

For Fig. 1(b) with a domain wall (10), we follow the discussion in Ref. 27 to show that such domain wall between phases with different Z_2 topological number possesses one Kramers pair of edge states at the boundary. In this case we consider

$$\tilde{H}(k_y) = E_0 + \begin{pmatrix} m & -ib_1\partial_x + (b_3 - ib_2)k_y \\ -ib_1\partial_x + (b_3 + ib_2)k_y & -m \\ & m & ib_1\partial_x - (b_3 + ib_2)k_y \\ ib_1\partial_x - (b_3 - ib_2)k_y & -m \end{pmatrix}. \quad (11)$$

To calculate the eigenstates it is convenient to perform unitary transformation as

$$H'(k_y) = Q^\dagger \tilde{H}(\vec{k}) Q = E_0 + \begin{pmatrix} b_2k_y & m - b_1\partial_x & & \\ m + b_1\partial_x & -b_2k_y & & \\ & & -b_2k_y & m - b_1\partial_x \\ m + b_1\partial_x & & b_2k_y & \end{pmatrix}, \quad (12)$$

where

$$Q = e^{-ib_3k_yx/b_1} \begin{pmatrix} 1 & 1 & & \\ i & -i & & \\ & & -i & -i \\ -1 & 1 & & \end{pmatrix}. \quad (13)$$

We omit the term E_0 henceforth, since it does not af-

fect the subsequent discussions. The eigenvalue problem reads as $H'(k_y)u_{k_y}(x) = E(k_y)u_{k_y}(x)$.

Because (12) is block-diagonal, we first solve the eigenvalue problem for the first two components of u_{k_y} , i.e we put $u_{k_y} = (u_1, u_2, 0, 0)^t$. We get

$$(E - b_2 k_y)u_1 = Du_2, \quad (14)$$

$$(E + b_2 k_y)u_2 = D^\dagger u_1, \quad (15)$$

where $D = m - b_1 \frac{\partial}{\partial x}$, $D^\dagger = m + b_1 \frac{\partial}{\partial x}$. They yield eigenequations for u_1 and u_2 , respectively:

$$DD^\dagger u_1 = (E^2 - b_2^2 k_y^2)u_1, \quad (16)$$

$$D^\dagger D u_2 = (E^2 - b_2^2 k_y^2)u_2, \quad (17)$$

When we solve Eq. (16) for u_1 , one can calculate u_2 from (15). As (16) is invariant under $E \rightarrow -E$, it seems that the solutions for E and $-E$ are always obtained simultaneously, namely there is a spectral symmetry between $E \leftrightarrow -E$. Nevertheless, it does not apply if $E = -b_2 k_y$, where (15) cannot be solved for u_2 . A similar situation occurs for $E = b_2 k_y$. Thus exceptions at $E = \pm b_2 k_y$ occur in the following way. For $u_1 (\neq 0)$ which satisfies $D^\dagger u_1 = 0$, we get $E = b_2 k_y$ and $u_2 = 0$ from Eqs. (14) and (15), whereas there is no solution with $E = -b_2 k_y$. In the same token, for u_2 which satisfies $D u_2 = 0$, we get $E = -b_2 k_y$ from (14), whereas there is no solution with $E = b_2 k_y$. Hence the spectral asymmetry is related to the kernels for D and D^\dagger . For simplicity we take $b_1 > 0$ henceforth, while the other case of $b_1 < 0$ can be studied in a similar way. For the domain wall (10), the solution of $D^\dagger u_1 = 0$ gives

$$u_1 \propto \exp\left(-b_1^{-1} \int^x m(s)ds\right) \quad (18)$$

and $E = b_2 k_y$, while $D u_2 = 0$ has no normalizable solution. Thus the energy dispersion in k_y direction has a branch $E = b_2 k_y$, which crosses the Fermi energy $E \sim 0$. This state is gapless, localized near $x = 0$.

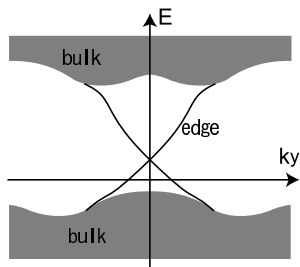


FIG. 2: Schematic dispersion curves for the model (11). Kramers theorem guarantees that the crossing of two edge states occur at $k_y = 0$.

So far we have solved the eigenequation for the first two components. The lower two components of the wavefunction u is obtained from above by time-reversal operation ($\Theta u(k_y) = i\sigma_2 u(-k_y)^*$). Therefore, the above-mentioned edge state with $E = b_2 k_y$ has a Kramers partner with $E = -b_2 k_y$. The whole dispersion is shown in Fig. 2. Thus we have shown that the Kramers pair of edge states exists at the boundary between the two phases. They cross at $k_y = 0$, as is guaranteed by the Kramers theorem.

IV. CONCLUSIONS

A general framework is established for classifying phase transitions between the quantum spin Hall and the insulator phases. For inversion-asymmetric systems, the phase transition accompanies a gap closing at $\vec{k} = \pm \vec{k}_0$ which is not at the high-symmetry points. For inversion-symmetric systems, the gap closes only at $\vec{k} = \vec{G}/2$ where \vec{G} is a reciprocal vector. All the known models exhibiting phase transition between the two phases are special cases of this general classification framework.

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¹ S. Murakami, N. Nagaosa, and S.-C. Zhang, *Science* **301**, 1348 (2003).

² J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, and A. H. MacDonald, *Phys. Rev. Lett.* **92**, 126603 (2004).

³ S. Murakami, N. Nagaosa, and S.-C. Zhang, *Phys. Rev. Lett.* **93**, 156804 (2004).

⁴ C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 146802 (2005).

⁵ C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* **95**, 226801

- (2005).
- ⁶ M. Onoda and N. Nagaosa, Phys. Rev. Lett. **95**, 106601 (2005).
 - ⁷ B. A. Bernevig and S.-C. Zhang, Phys. Rev. Lett. **96**, 106802 (2006).
 - ⁸ X.-L. Qi, Y.-S. Wu and S.-C. Zhang, Phys. Rev. B **74**, 085308 (2006).
 - ⁹ D. N. Sheng, Z. Y. Weng, L. Sheng, and F. D. M. Haldane, Phys. Rev. Lett. **97**, 036808 (2006).
 - ¹⁰ T. Fukui and Y. Hatsugai, Phys. Rev. B **75**, 121403(R) (2007).
 - ¹¹ L. Fu and C. L. Kane, Phys. Rev. B **74**, 195312 (2006).
 - ¹² L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007).
 - ¹³ L. Fu and C. L. Kane, Phys. Rev. B **76**, 045302 (2007).
 - ¹⁴ S. Murakami, Phys. Rev. Lett. **97**, 236805 (2006).
 - ¹⁵ M. Onoda, Y. Avishai, N. Nagaosa, Phys. Rev. Lett. **98**, 076802 (2007).
 - ¹⁶ C. Wu, B. A. Bernevig, and S.-C. Zhang, Phys. Rev. Lett. **96**, 106401 (2006).
 - ¹⁷ C. Xu and J. E. Moore, Phys. Rev. B **73**, 045322 (2006).
 - ¹⁸ B. A. Bernevig, T. L. Hughes, S.-C. Zhang, Science **314**, 1757 (2006).
 - ¹⁹ S. Murakami, New J. Phys. **9**, 356 (2007).
 - ²⁰ The pseudospin α , which labels the eigenstates, is different from the spin in the presence of the spin-orbit coupling.
 - ²¹ V. J. von Neumann and E. Wigner, Physik. Zeitschr. **30**, 467 (1929).
 - ²² J. E. Avron, L. Sadun, J. Segert, and B. Simon, Phys. Rev. Lett. **61**, 1329 (1988).
 - ²³ J. E. Avron, L. Sadun, J. Segert, and B. Simon, Commun. Math. Phys. **124**, 595 (1989).
 - ²⁴ By considering all possible 2D magnetic point groups, we found some exceptional models with degeneracy at $\vec{k} = \vec{G}/2$, even without I-symmetry. These cases result from a rather high symmetry of the system. It is expected that by including some perturbation to lower the symmetry the Hamiltonian will reduce to the case (a) in Fig. 1.
 - ²⁵ In some exceptional cases with high point-group symmetry, the gap between two doubly degenerate bands can close even when $\vec{k} \neq \vec{G}/2$. In 2D this occurs for the magnetic point-group symmetries $\bar{3}'$, $\bar{3}'m$, $\bar{3}'m'$, $6'/m$, $6'/mm'm$, which are in trigonal system or hexagonal systems. It is expected that the closing of the gap in these cases does not correspond to phase transition between the QSH and the SHI, as some perturbation can circumvent this degeneracy.
 - ²⁶ J. E. Moore and L. Balents, Phys. Rev. B **75**, 121306(R) (2007).
 - ²⁷ A similar problem has been discussed in the context of fractional fermion number. See A. J. Niemi and G. W. Semenoff, Phys. Rep. **135**, 99 (1986) for a review. A concrete example is the midgap state associated with dimerized soliton in polyacetylene as discussed in W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).